

Validation of 3-D Commercial Codes for Microfluidic Systems



Klint A. Rose
(925) 423-1926
rose38@llnl.gov

The fabrication and testing of micro-fabricated structures is very expensive and time consuming. Using model-driven methods, we can reduce the number of iterations and cover the large configuration space of microfabricated structures in an effective and affordable manner. Specifically, we validate the modeling tools against microfluidic structures focused at performing front-end sample preparation for biological assays.

Project Goals

Our goal is to implement a general, multiphysics simulation capability for use as a predictive tool for microfluidic systems.

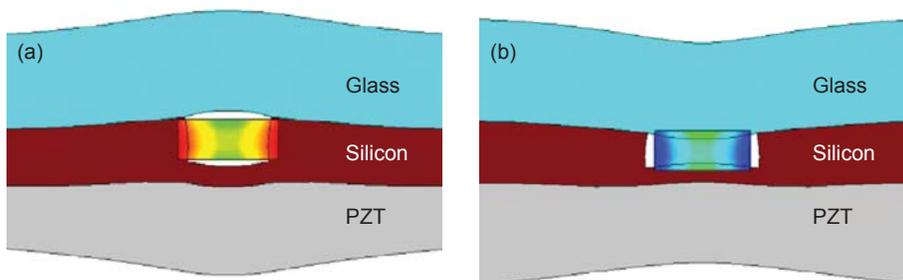


Figure 1. Example of the pressure fields generated in a fluid volume (fixed rectangular center) by a glass-silicon-PZT stack: (a) high pressures (red) generated at the edges of the fluid volume as the sidewalls compress inward; (b) low pressures (blue) generated at fluid volume edges as the sidewalls expand outward.

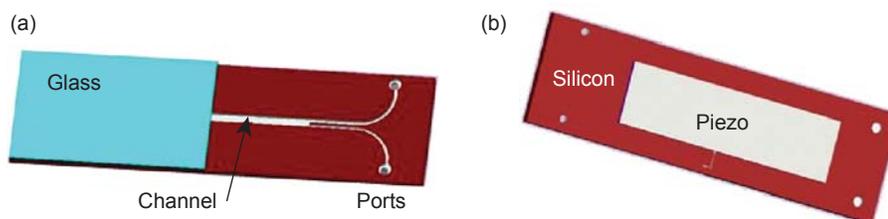


Figure 2. CAD drawing of the microfluidic chip used to validate the simulation: (a) front view of chip showing the glass top and bifurcated separation channel etched into the silicon base; (b) bottom view of the chip showing the PZT.

Relevance to LLNL Mission

The rapid identification of emerging viruses is critical to national security and financial health. Of the 80 emerging pathogens identified since 1980, 59 have been viruses. A common failure mode in biological detection systems is the high false negative rate for viruses because of their large mutation rate, small size, and lack of adequate automated sample preparation instrumentation. Microfluidic technology is ideally suited to improve sample preparation and aid in virus discovery. However, improved modeling tools are required to accelerate the understanding of microfluidic systems when applied to high-throughput front-end sample preparation systems.

FY2008 Accomplishments and Results

We describe a modeling approach used to capture the particle motion within an acoustic focusing microfluidic device. Our approach combines finite element models (FEM) for the acoustic forces with analytical models for the fluid motion and using these force fields to calculate the particle motion in a Brownian dynamics simulation.

Acoustic focusing is an effective technique to manipulate relatively large ($> 2 \mu\text{m}$) particles and has been used for a variety of applications including sorting blood cells, concentrating cells for optical detection, and measuring particle zeta potentials.

By focusing large contaminants into a single plane or node within the micro-channel, we can separate a complex input sample into waste and purified streams and direct each to separate outputs. The location and width of the focused particle band depends on the

channel geometry, material properties, and acoustic transducer operating conditions. The transducer generates pressure fields within the microchannel (Fig. 1) creating acoustic radiation forces whose direction and magnitude depend on the relative compressibility and density of the particle and the fluid. Currently, models predicting net particle motion within acoustically driven devices rely on simplified 1-D models for the acoustic forces. FEM simulations have been used to analyze the 2-D force field in a microfluidic device, but this analysis provides only qualitative information regarding the likely particle locations.

In our approach, we solve for the hydrodynamic flow field using analytical solutions based on the geometry of the microchannel and solve for the 2-D acoustic force field within the channel using a commercial FEM code (ATILA FEA). We incorporate the force fields into a Brownian dynamics simulation based on the Langevin equation. This simulation includes random displacements due to Brownian motion and calculates spatial and temporal concentration distributions for any species within the device.

To validate the model we experimentally measured the degree of focusing (full width half maximum) for microspheres with diameters ranging from 1 to 5 μm . We used a microfluidic chip, shown in Fig. 2, with channels etched into a silicon wafer and a piezo-electric transducer (PZT) glued to the backside at a frequency of 1.46 MHz and an input voltage from 0 to 9.6 V. The 2-D force field we predicted for these conditions (Fig. 3) suggests a single node in the lower center region of the channel.

Experimental and simulated results for the width of the focused particle band, shown in Fig. 4, compare favorably across particle sizes and driving voltages when the simulated values are scaled by a factor of 40. This result demonstrates our ability to qualitatively capture the acoustic focusing force magnitudes and directions versus the input flow rates and random particle motion.

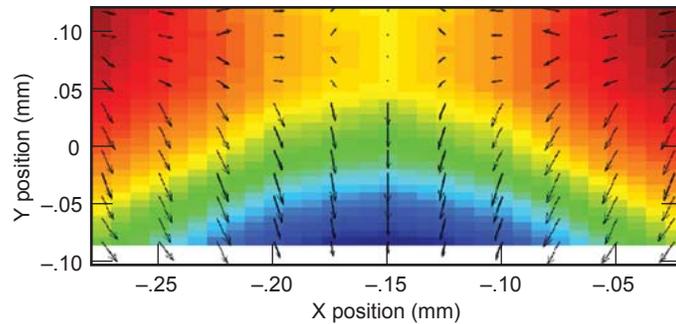


Figure 3. Simulated result for the acoustic radiation force field in the microfluidic chip cross-section when the PZT is driven at 1.46 MHz. The map indicates the high (red) to low (blue) pressure field. Arrows show the direction of the acoustic forces.

Related References

1. Kapishnikov, S., V. Kantsler, and V. Steinberg, "Continuous Particle Size Separation and Size Sorting Using Ultrasound in a Microchannel," *Journal of Statistical Mechanics*, P01012, 2006.
2. Zhou, C., P. Pivarnik, A. G. Rand, and S. V. Letcher, "Acoustic Standing-Wave Enhancement of a Fiber-Optic Salmonella Biosensor," *Biosensors & Bioelectronics*, **13**, pp. 495–500, 1998.
3. Hunter, R. J., and R. W. O'Brien, "Electroacoustic Characterization of Colloids with Unusual Particle Properties," *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, **126**, pp. 123–128, 1997.
4. Nyborg, W. L., "Radiation Pressure on a Small Rigid Sphere," *Journal of the Acoustical Society of America*, **42**, 5, p. 947, 1967.
5. Martyn H., Y. Shen, and J. J. Hawkes, "Modeling of Layered Resonators for Ultrasonic Separation," *Ultrasonics*, **40**, pp. 385–392, 2002.

FY2009 Proposed Work

Our future work will aim to eliminate the need for a scaling factor by modeling the full 3-D force field and including losses due to material interfaces.

Using the methodology described here, we can rapidly iterate over a variety of input parameters including geometry, acoustic driving voltage and frequency, and particle properties to predict the spatial and temporal particle concentration distributions within a microfluidic device and achieve an optimized system configuration.

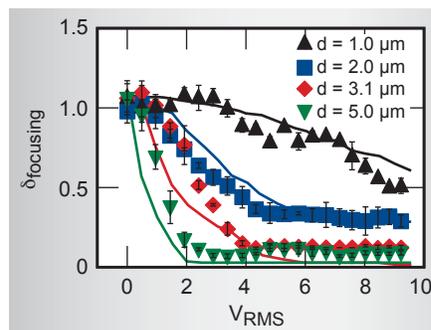


Figure 4. Comparison of experimental and theoretical measurements. The solid lines show the theoretical force field predicted from the simulations; the symbols indicate the experimental values.